

Designing for  
High-Precision  
Lattice QCD

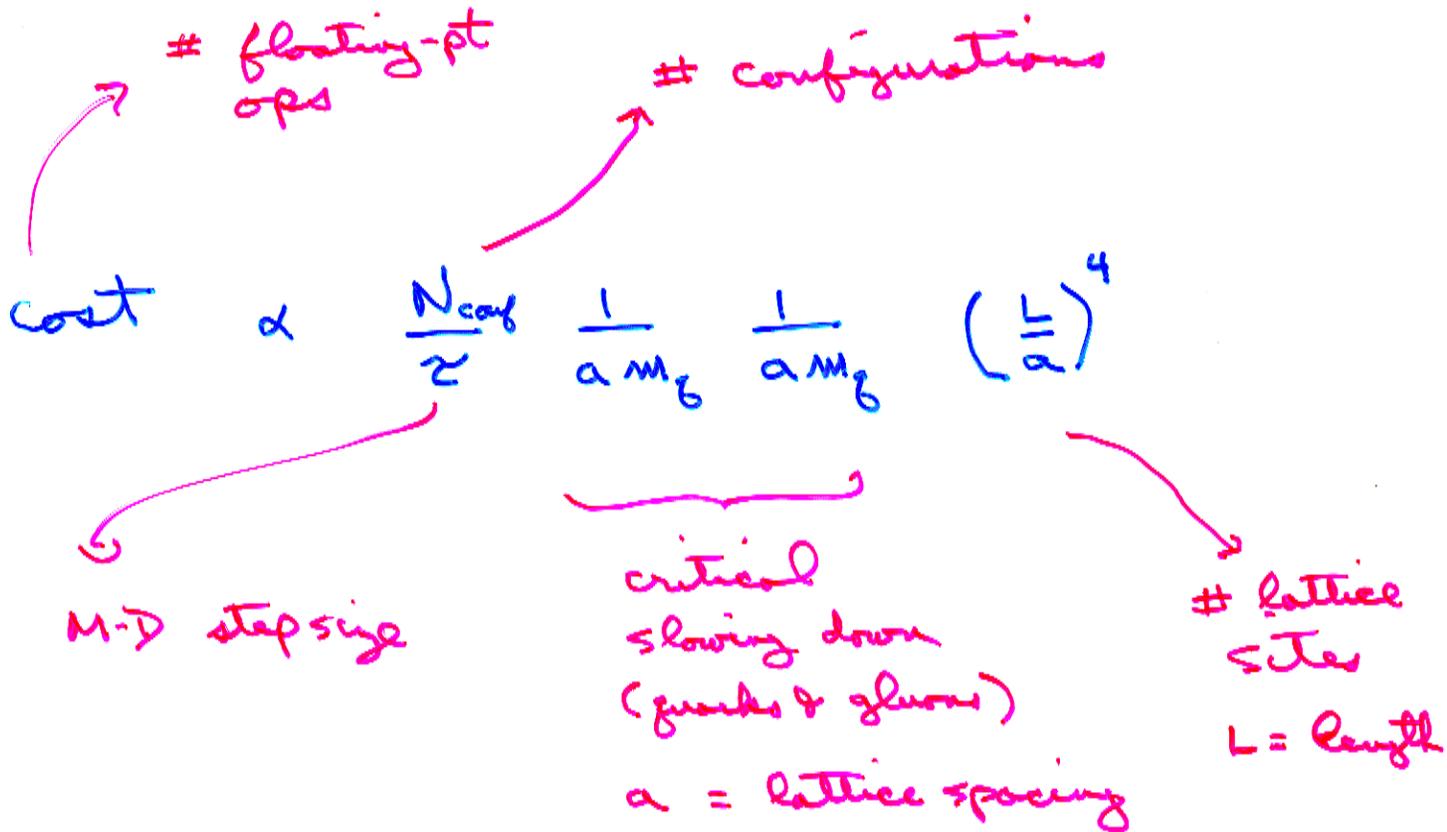
G.P. Lepage

3/26/01

# History: Fall & Rise of LQCD

- invented 1974; "explains" confinement
- stalls for almost 20 yrs
  - Ken Wilson declares it dead (1989)
- renaissance in 1990's
  - Parton theory fixed
  - eff. field theories for c, b's (NRQCD, HW, HQET...)
  - improved discretizations
    - ⇒ larger lattice spacings
- 1<sup>st</sup> high-precision nonpert'v results
  - $\alpha_s(M_Z)$ ,  $M_G$  ... to few %
  - Ken Wilson retracts (~1995)

# Cost - Error Analysis



NB Cost  $\propto (1/a)^6$  is highly dependent on  $a$

$\Rightarrow$  keep  $a$  as large as possible.

NB Cost  $\propto (1/a)^{10\dots}$  for other problems

Several sources of error.

Optimum  $\Rightarrow$

all errors roughly equal  
to each other ( $\approx \epsilon$ )

## Sources (current practice):

- statistical:  $\varepsilon \propto 1/\sqrt{N_{\text{conf}}}$   $\Rightarrow$   $N_{\text{conf}} \propto \varepsilon^{-2}$
- finite  $a$ :  $\varepsilon \propto a^2$   $\Rightarrow$   $a \propto \varepsilon^{1/2}$
- finite  $\tau$ :  $\varepsilon \propto \tau^2$   $\Rightarrow$   $\tau \propto \varepsilon^{1/2}$
- $m_b$  extrop'n:  $\varepsilon \propto m_b^{1.5}$   $\Rightarrow$   $m_b \propto \varepsilon^{2/3}$
- finite  $L \Rightarrow$  log. effect (ignore)

substitute in cost formula  
to relate cost  $\leftrightarrow \varepsilon$

⇒

$$\text{Error } \epsilon \propto (1/\text{cost})^{1/\omega}$$

$$\text{where } \omega = 6\frac{5}{6} \approx 7$$

⇒ 10-fold increase in computer  
reduces errors by only 29%  
(100-fold ⇒ 49% reduction)

⇒ high-precision LQCD cannot  
be achieved solely through  
larger computers

Algorithm improvement is essential to high-precision LQCD

NB

- $\omega = 10$  in 1980's (Wilson quarks)

$\Rightarrow$  even worse than above

- LQCD revolution in 1990's was an algorithmic revol'n not a hardware revol'n.

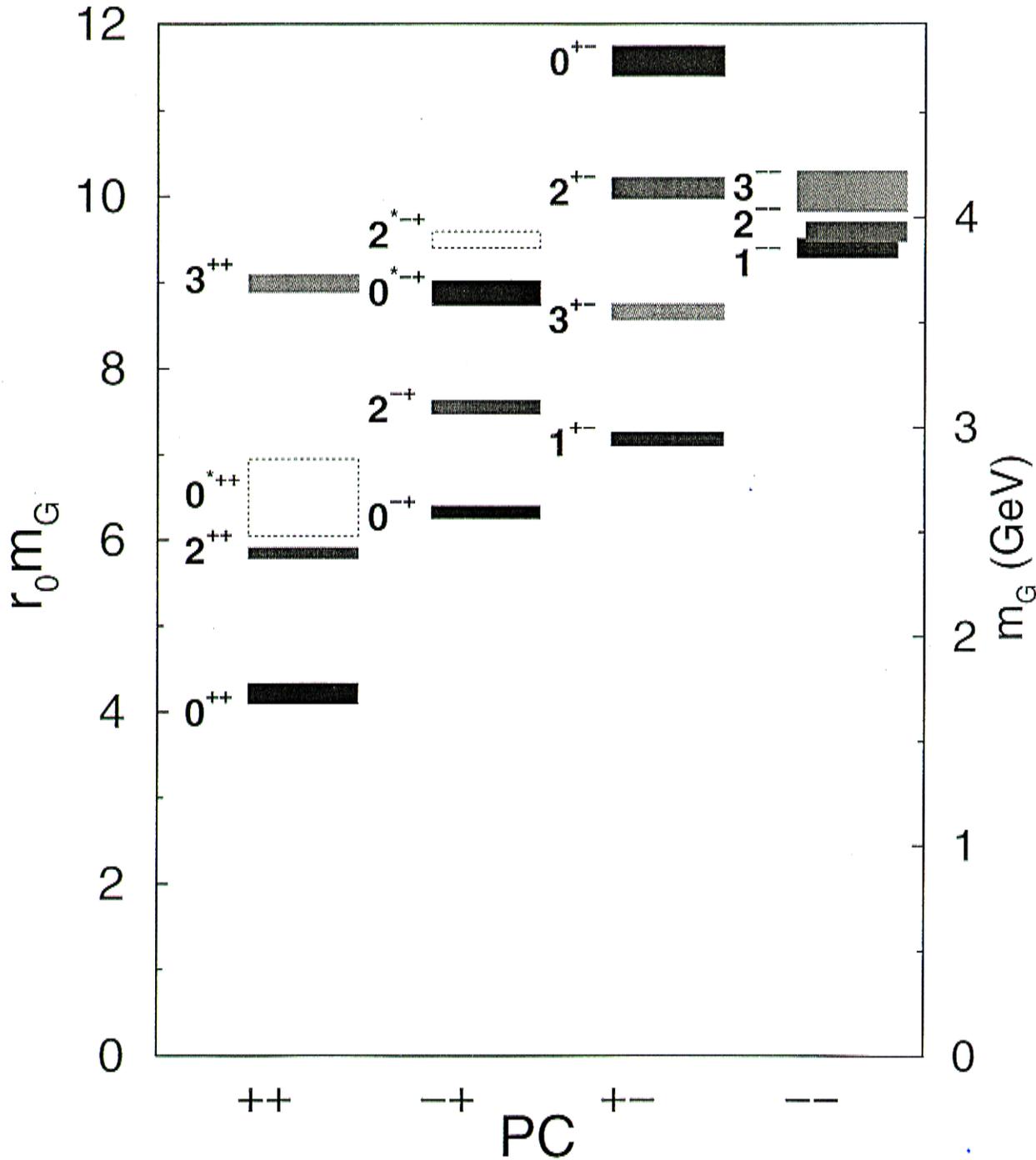
eg) glueballs

10-100x better

with  $\frac{1}{100}$  hardware

# Glueball Spectrum

( $n_f=0$  QCD)



Morrongiata  
& Pearson  
1998

## Improved Discretizations

finite element errors biggest  
problem  $\Rightarrow$  need improved  
discretizations.

- lowers  $\omega$  a little
- lowers prefactor a lot

$$\text{in } \varepsilon \times (\text{cost})^{1/3}$$

# Gluons

Std. gluon Lagrangian (Wilson)

$\Rightarrow \mathcal{O}(a^2)$  errors

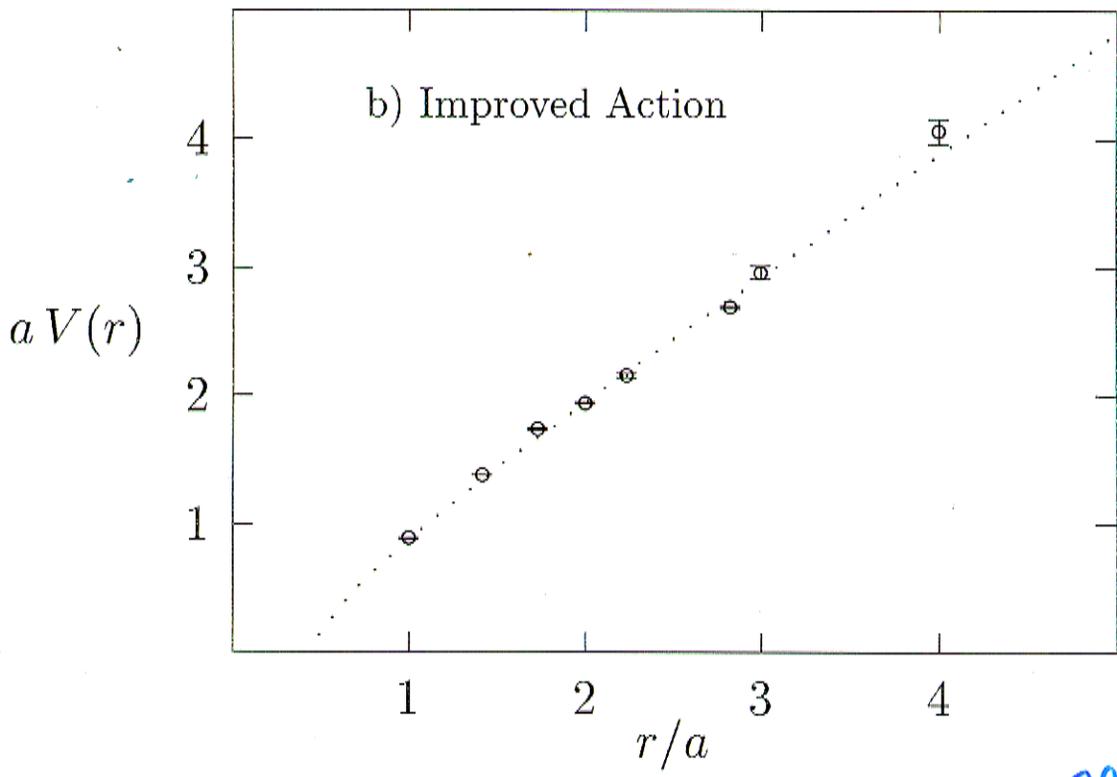
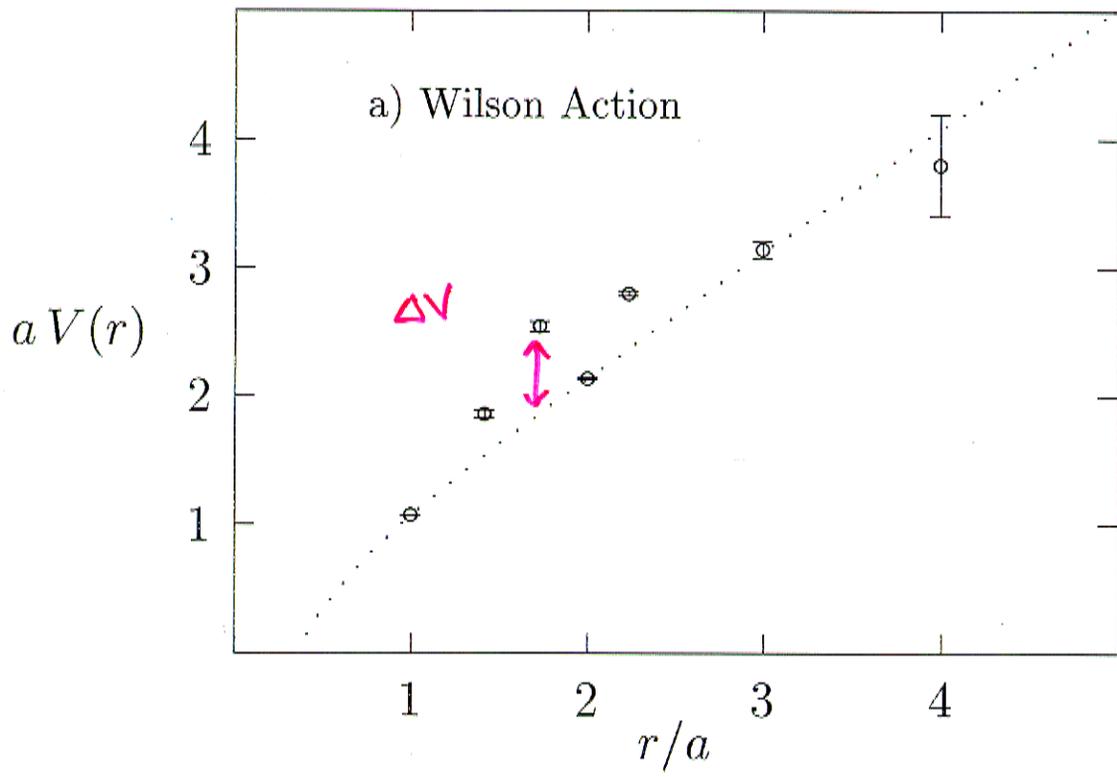
$$L_{\text{Wilson}} \rightarrow -\frac{1}{2} \text{Tr} F_{\mu\nu} F^{\mu\nu}$$

$$+ d a^2 \sum_{\mu\nu} (\mathcal{D}_\mu F_{\nu\rho})^2$$

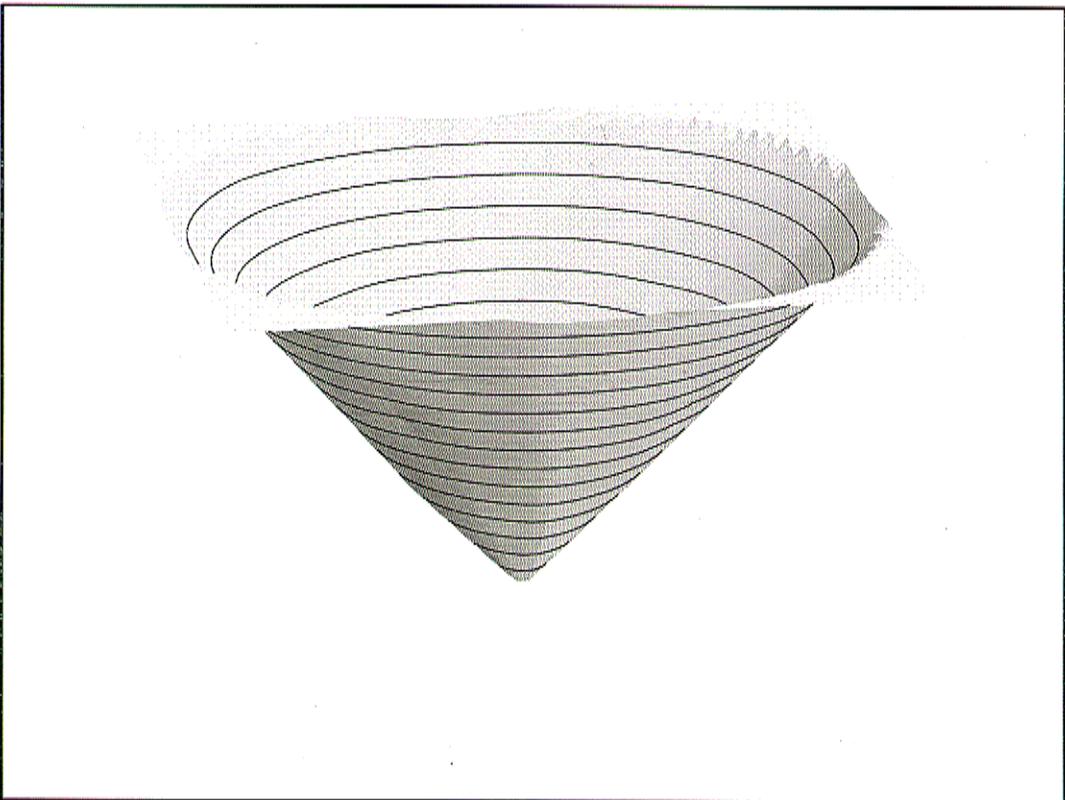
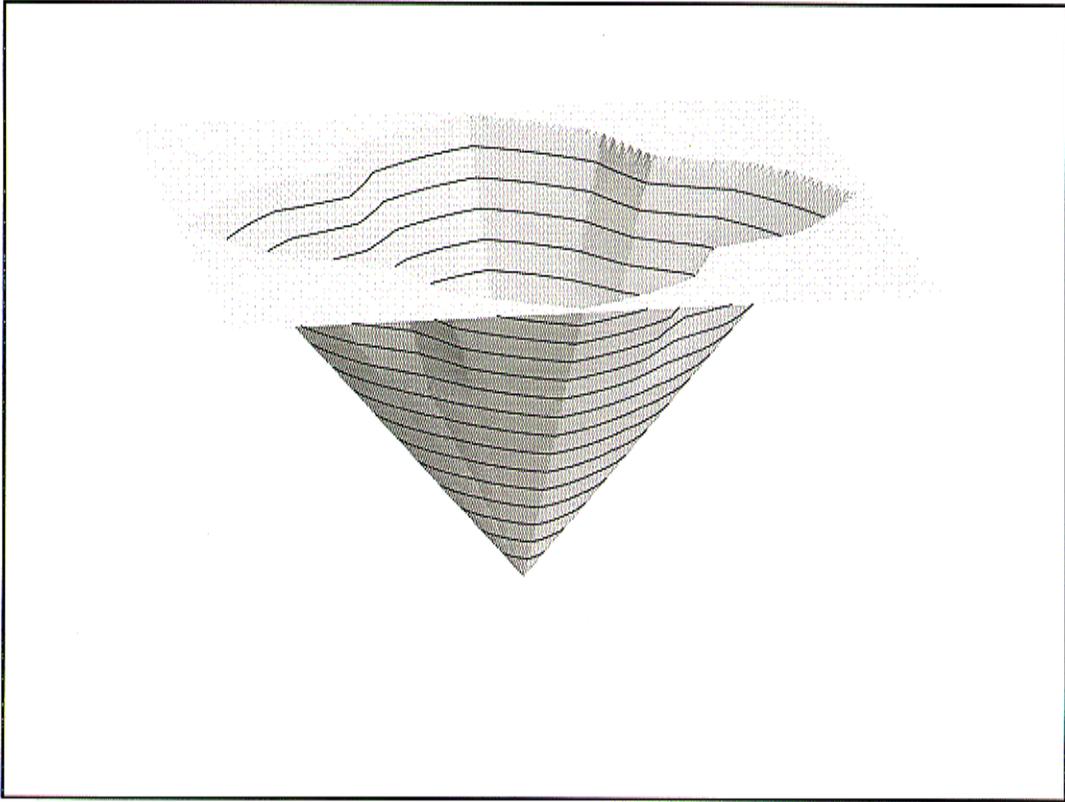
+ ...

not Loc. inv! +

remove with improved discretization



Alford et al  
~ 1975



## Light Quarks (u, d, s)

Std lattice formalisms  $\Rightarrow$   $\mathcal{O}(a, a^2)$   
error

$$\mathcal{L}_0 \rightarrow \bar{\Psi} (\mathcal{D}_m \gamma_m + m) \Psi$$

$$+ c(a) a^2 \bar{\Psi} (\mathcal{D}_m^3 \gamma_m) \Psi$$

+ ...

$\rightarrow$  remove with improved discretization.

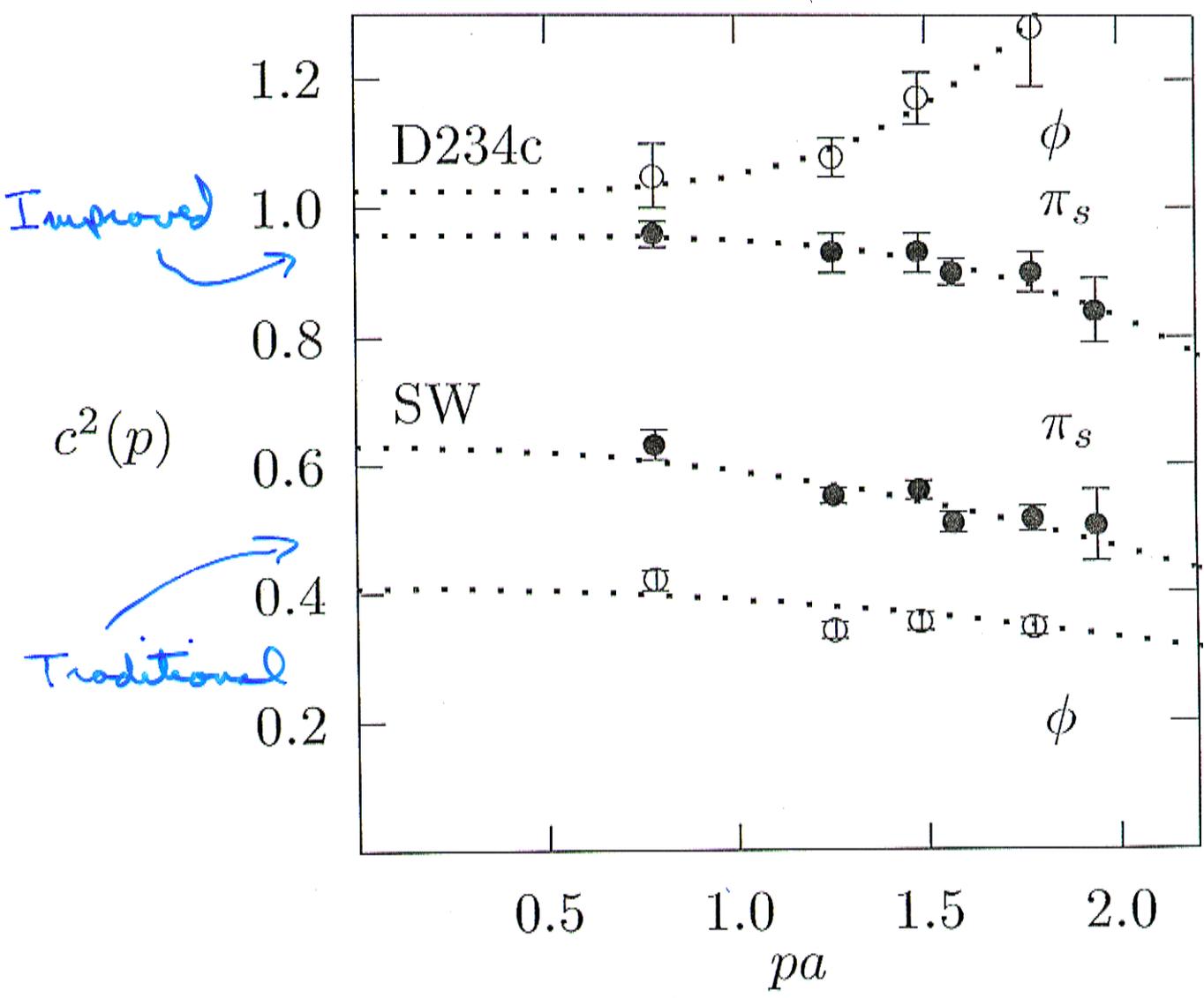
$$a^2 \text{ error} \sim \sum \frac{a^2}{6} D_\mu^3 \delta_\mu$$

$\Rightarrow$  breaks hor. inv'ce

Test by computing

$$c^2(p) = \frac{E_\pi^2(p) - m_\pi^2}{\vec{p}^2}$$

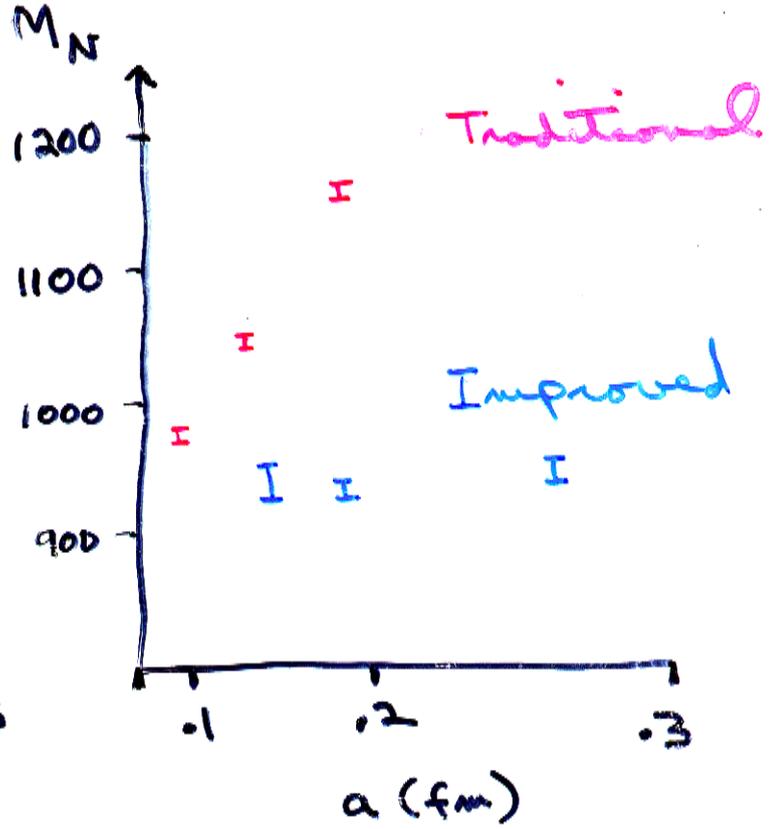
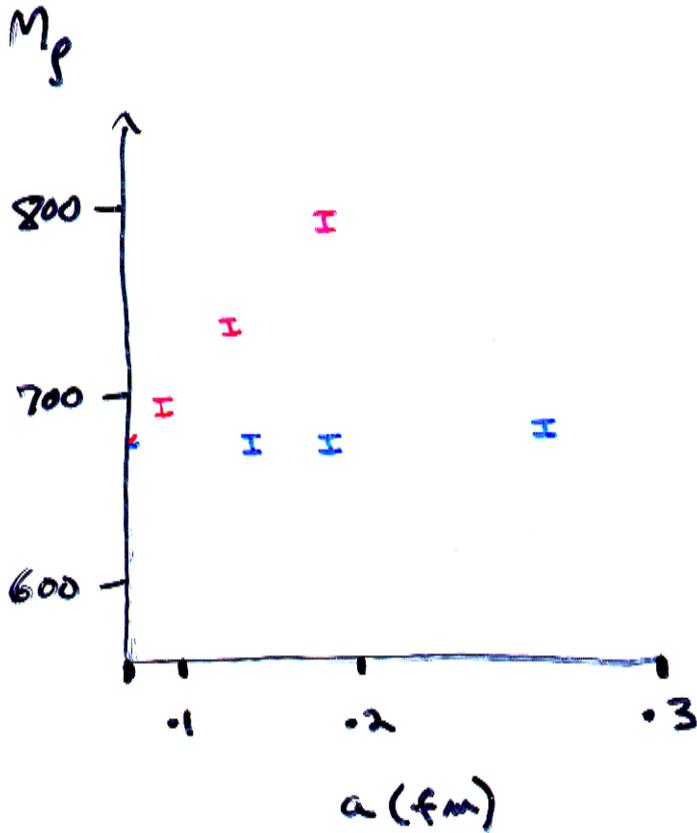
= 1  $\forall p$  if  
relativity correct.



$$c^2(p) = \frac{E^2(p) - m^2}{\vec{p}^2}$$

$$= 1 \quad \forall p \quad \text{if relativity correct}$$

# Staggered-Quarks: a independent?



MILC  
Collab'n  
12/99  
(GRL 1998)

# QFT Numerical Analysis

QFT  $\Rightarrow$  important structure  
at arbitrarily short  
distances

$\Rightarrow$  ordinary numerical  
analysis "renormalized"

$\hookrightarrow$  to account for  
effects of structure  
smaller than grid  
spacing  $a$ .

es)

$$\frac{\partial \psi(x)}{\partial x} \rightarrow \Delta \psi(x) + c(a) a^2 \Delta^3 \psi + \dots$$

$$\frac{\psi(x+a) - \psi(x-a)}{2a}$$

$$-\frac{1}{6} + c_1 a_s \left(\frac{\pi}{a}\right) + c_2 a_s^2 + \dots$$

Numerical  
Analysis

Renormalization  
→ context specific  
→ calculable  
with Padé  
if a small  
enough.

Problem before 1990's :

Part in th. didn't work  
at all for reasonable a's

↳ Technical problem  
fixed in 1990's.

eg) Wave fun at origin ( $f_B, \Gamma_{ee} \dots$ )

$$\Psi_{\text{true}}(0) = \sum \Psi_{\text{ext}}(0) + \eta a^2 \nabla^2 \Psi_{\text{ext}} + \dots$$

$1 + \alpha_S + \alpha_S^2 \dots$

$\Rightarrow$  need pert. theory (or equiv.)  
even if not improving  
discretization.

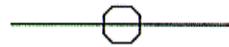
## Present Status

- 10-30% accurate results for a wide range of masses, decay constants, form factors .....

↳ Major advance, mostly since 1995.

$f_{B_s}$  in MeV

NRQCD '98



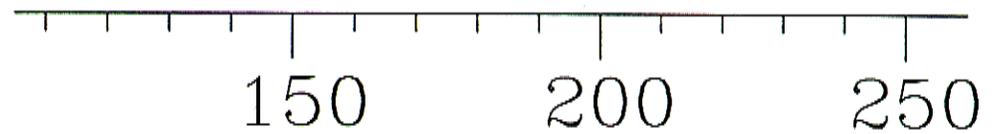
Fermilab '97

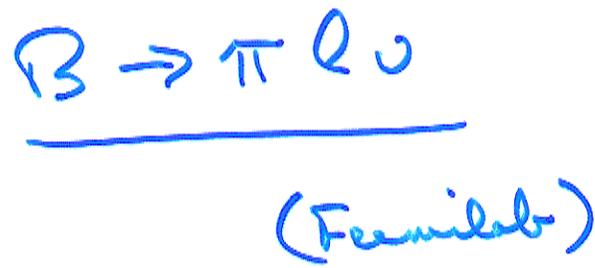


JLQCD '97



MILC '97





$\Rightarrow V_{ub}$

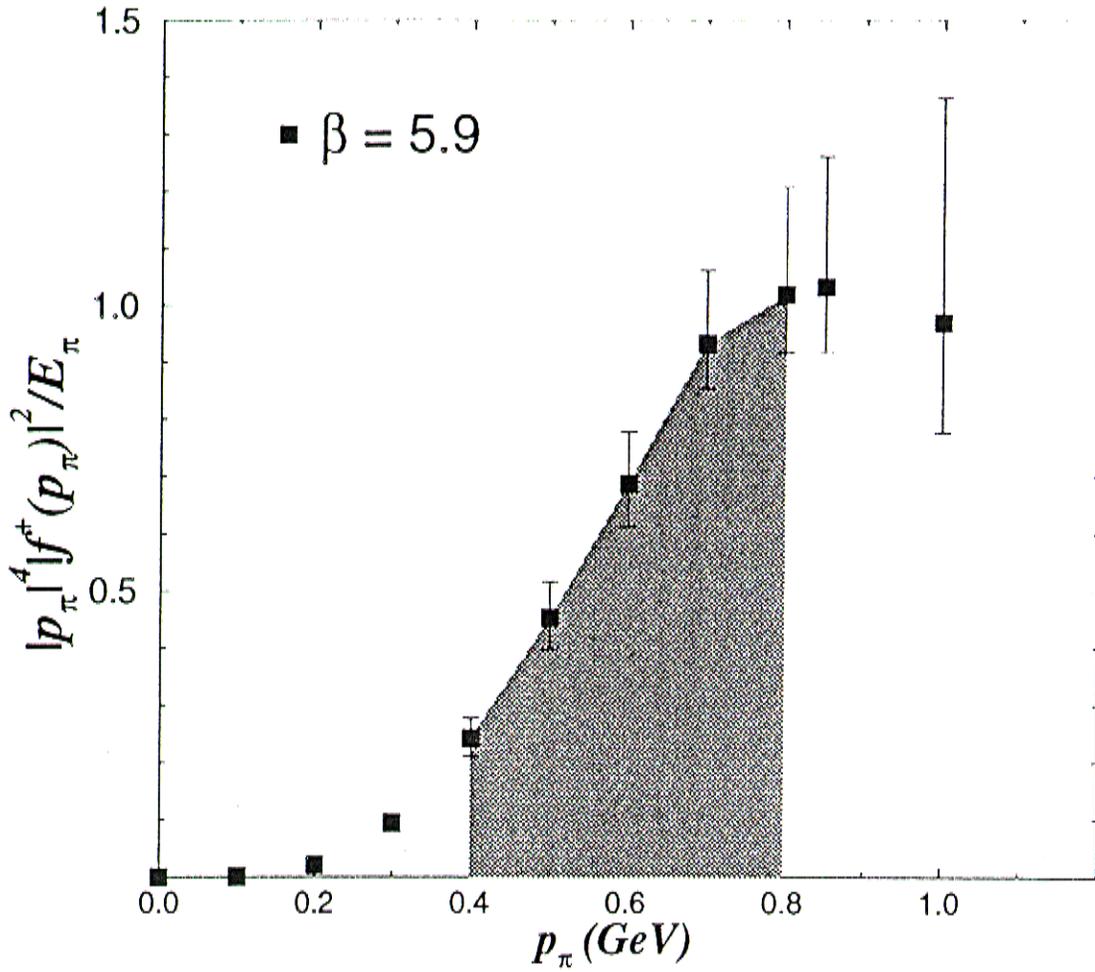


Figure 3. Differential decay rate at  $\beta = 5.9$  and partial width

## Near-Term Future (2-4 yrs)

- 1% accurate results for  $f_B, B_B, \Gamma(B \rightarrow \pi \ell \nu)$  ..... essential to exp'l programs at CLEO/CLEO-C, BaBar KEK .....
- Cornell Workshop (Jan 2001)  
 $\Rightarrow \sim 1\%$  accuracy possible  
now for dozens of "gold-plated" calculations on  $\frac{1}{2}$  - 1 TF commodity cluster
  - aggressive use of PTH & improved disc.
  - larger lattice spacing:  $a = .1 - .4 \text{ fm}$
  - includes  $f_B, B_B, B \rightarrow \pi \ell \nu$  .....
  - want lattice results before exp'l results

# Design Issues

## Rapid Modifications

- despite its size, lattice QCD is still in its infancy
  - ⇒ methods change rapidly
  - ⇒ hardware/software must be able to track changes
- elaborate optimization of hardware/software for specific discretizations/algorithms is a mistake.
  - focus on low-level components
    - $SU_3$  multiply ✓
    - Dirac operator ? X

## Rich Software Development Environment

- improved algorithms/disc's are more complicated and change often
- need standard power tools for code development: debuggers, profilers, C++, Python ----
- must be easy to change  
⇒ reduces barrier to innovation (innovation is still essential).

Eg

```
Matrix wloop(int L,int T,const Linkfield& U)
{
  // computes LxT wilson loop
  const Grid& g = U.grid();
  Dir mu(g),nu(g);
  Site x(g);
  Matrix w=0;
  for_all(mu)
    for_all(nu) if(mu!=nu)
      {
        Path p = L*mu+T*nu-L*mu-T*nu;
        for_all(x)
          w += U(x,p);
      }
  w = 0.5*(w+conj(w));
  return w/g.nsite()/(g.ndir()*g.ndir()-1);
}
```

↳ worth a factor of 2  
in performance

## Flexible Communications

Improved algorithms / discretizations  
are less local or even non-local

Eg) improved staggered quarks  
have 3<sup>rd</sup>-nearest neighbor  
interactions

Eg) FFT's essential for  
high- $\beta$  runs used  
for  $\geq 3$ -loop P.T.h.

## Support for Small Lattices

- lattice QCD hardware often optimized for large lattices :  $L \approx 32, 64, 128, \dots$
- improved discretization  
 $\Rightarrow a = 0.1 - 0.4 \text{ fm}$   
 $\Rightarrow \text{need } L \approx 6, 9, 12, 18, 24$
- partition machine for multiple simulations at same time  
 $\Rightarrow$  10 TF facility  
    = 10 x 1 TF clusters  
    (scalability)

$$\cancel{cf} \quad \varepsilon \propto \left(\frac{1}{\cos t}\right)^{1/7}$$

## Rapid Turnaround for R&D

Big computers essential for

- algorithm development & testing
  - analysis
  - part'n theory (|| vegas)
- } feedback  
in ~ 1 day  
eg) ACPMAPS

⇒ production machines must  
be sufficiently flexible  
to handle such tasks

↳ easy software essential

# Design Summary

- Rapid Modifications : LQCD still changing
- Rich Software Development Environ.
- Flexible Communications : support non local algorithms (eg FFT)
- Small Lattices : partition for  $L = 6, 9, \dots$
- Rapid Turnaround for R&D : production machines for R&D, partitioning ...